

# Competition of isoscalar and isovector proton-neutron pairing in nuclei

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We use shell model techniques in the complete  $pf$  shell to study pair correlations in nuclei. Particular attention is paid to the competition of isoscalar and isovector proton-neutron pairing modes which is investigated in the odd-odd  $N = Z$  nucleus  $^{46}\text{V}$  and in the chain of even Fe-isotopes. We confirm the dominance of isovector pairing in the ground states. An inspection of the level density and pair correlation strength in  $^{46}\text{V}$ , however, shows the increasing relative importance of isoscalar correlations with increasing excitation energy. In the Fe-isotopes we find the expected strong dependence of the isovector pairing strength on the neutron excess, while the dominant  $J = 1$  isoscalar pair correlations scale much more gently with neutron number. We demonstrate that the isoscalar pair correlations depend strongly on the spin-orbit splitting.

21.10-k, 21.60.Fw, 21.60.Ka

## I. INTRODUCTION AND MOTIVATION

Stimulated by progress in many-body theories and the advent of novel experimental tools like the radioactive ion-beam facilities, pairing in nuclei, and in particular proton-neutron ( $pn$ ) pairing, has become quite fashionable recently [1–10]. In contrast to like-nucleon pairing,  $pn$  pairing may exist in two distinct varieties - isovector and isoscalar pairing. Isovector  $pn$  pairing has been found to decrease fast with increasing neutron excess (or more precisely with increasing  $|N - Z|$ , where  $N, Z$  are the numbers of neutrons and protons, respectively) within an isotope chain [1]. Thus, it is obvious that  $pn$  pairing is relatively more important in  $N = Z$  nuclei. While even-even  $N = Z$  nuclei have ground state isospin  $T = 0$  and isospin symmetry forces isovector pairing to be identical in all three  $T = 1$  pairing channels (proton-proton ( $pp$ ), neutron-neutron ( $nn$ ), and proton-neutron), this symmetry is broken in most odd-odd  $N = Z$  nuclei with mass number  $A > 40$  which have  $T = 1$  ground states. Indeed, it is observed that isovector  $pn$  pairing is the dominating pairing mode in these nuclei. On the other hand, odd-odd  $N = Z$  nuclei with  $A < 40$  have ground state isospin  $T = 0$  (with the only exception of  $^{34}\text{Cl}$ ) pointing to a competition between the two different  $pn$  pairing modes and its change with mass number is an obvious source of interest. The interplay of isovector and isoscalar  $pn$  pairing has been studied in various contexts:

- It has long been known that  $N = Z$  nuclei gain extra binding compared to the smooth trend defined by their neighbors. This extra piece, called the Wigner energy, is stronger for even-even than for odd-odd nuclei. Recent studies of the Wigner energy tried to relate its origin to the  $pn$  pairing [11].
- Odd-odd  $N = Z$  nuclei are the only ones with two nearly degenerate low-lying isospin states ( $T = 0$

and  $T = 1$ ). This fact and the change of the ground state isospin from  $T = 0$  to  $T = 1$  at  $A = 40$  has been explained by a near balance of isovector pairing and symmetry energy [10].

- While the ground state isospin of odd-odd  $N = Z$  nuclei with  $A > 40$  (except for  $^{58}\text{Cu}$ ) is  $T = 1$ , it is experimentally found that the density of  $T = 0$  levels at modest excitation energies is larger than the density of  $T = 1$  states. For example, for  $^{74}\text{Rb}$  a transition from isovector to isoscalar dominance has recently been observed with increasing rotational frequency [12]. This transition has been traced back to a competition between isovector  $J = 0$   $pn$  pairing and isoscalar aligned  $pn$  pairing ( $J = 9$ ), where the latter becomes obviously more important at larger angular momenta [13].

The interplay and competition of isovector and isoscalar pairing is also the theme of this paper, where we study and discuss two different aspects of this topic. At first, we perform detailed studies of the spectrum of  $^{46}\text{V}$ . Special emphasis is paid to the comparison of the  $T = 0$  and  $T = 1$  parts of the spectra and their dependence on the pair correlation strength. In particular, we investigate the temperature dependence of the various pairing modes tracing possible differences in the behavior of the isovector and isoscalar  $pn$  pairing.

Isovector pairing in the dominating  $J = 0$  channel involves coupling of states in time-reversed components of the same orbitals. Very often isovector pairing is effectively given by one single matrix element describing the  $J = 0$  pairing of the valence nucleons in one partly filled orbital (the  $f_{7/2}$  orbital in the nuclei studied in this paper). In contrast, isoscalar  $pn$  pairing, even its  $L = 0$  component, can involve not only pairing within the same orbital, but also between spin-orbit partners.

Thus isoscalar  $pn$  pairing involves several scales: the coupling matrix element(s) in the same orbital, the usually strong (e.g.  $J = 1$ ) matrix element between spin-orbit partners, and finally the spin-orbit splitting which can be understood as a penalty which reduces this otherwise very favorable correlation. To shed some light on the importance of isovector versus isoscalar pairing, and in particular, on the role played by the spin-orbit splitting we study pair correlations within the even Fe-isotopes  $^{50-56}\text{Fe}$  comparing the results of “realistic calculations” to those in which we have artificially reduced the spin-orbit splitting.

Our studies have become feasible due to recent progress made in solving the interacting shell model, which is the method of choice to investigate correlations among nucleons. All calculations are performed with the realistic KB3 interaction [14] in the complete  $pf$  shell. Modern diagonalization codes allow now studies in model spaces whose dimensions have been considered untractable only a few years ago. We use such a state-of-the-art diagonalization code [15] in our calculation of  $^{46}\text{V}$  and hence have the possibility to study the spectrum and its properties in a state-by-state approach. About a year ago, when we started our investigations of pairing properties in the Fe-isotopes, diagonalization codes seemed not to be able to handle valence model spaces of these dimensions (for very recent progress, the reader is referred to [16]). For that reason we have adopted the Shell Model Monte Carlo (SMMC) approach [17–19] for these studies. In the SMMC the nucleus is described by a canonical ensemble at finite temperature. Since the Monte Carlo techniques avoid an explicit enumeration of the many-body states, they can be used in model spaces far larger than those accessible to conventional diagonalization methods. As a disadvantage compared to these methods, the SMMC approach cannot study detailed spectroscopy and ground state properties are achieved as the limit of low temperatures. To circumvent the “sign problem” encountered in the SMMC calculations, we adopt the “g-extrapolation” procedure suggested in Ref. [20].

Both methods - the diagonalization approach and the SMMC - are well documented in the literature and thus there is no need for a repetition here. For detailed descriptions of the methods we refer the reader to [19,21].

## II. RESULTS AND DISCUSSION

First we discuss results obtained for the odd-odd  $N = Z$  nucleus  $^{46}\text{V}$  by diagonalization in the complete  $pf$  shell. The calculated spectrum is compared to the experimental spectrum [22] in Fig. 1. We find overall good agreement, although the calculated  $T = 0$  spectrum is at slightly too low (by about 400 keV) excitation energy.

Given the spectrum of the nucleus, we define the internal energy at a finite temperature  $T$  by ( $\beta = 1/T$ )

$$U(T) = \frac{1}{Z} \sum_i (2J_i + 1) E_i \exp[-\beta E_i] \quad (1)$$

with the partition function

$$Z = \sum_i (2J_i + 1) \exp[-\beta E_i]; \quad (2)$$

the sums runs over all nuclear levels  $i$  labeled by quantum numbers  $(T_i, J_i)$  and excitation energy  $E_i$ . Fig. 2 displays the internal energy and the specific heat  $C_v = \frac{d}{dT}U(T)$  as function of temperature  $T$ . The striking feature is the double-peak structure in the specific heat. While the peak around  $T = 1.5$  MeV is trivially related to the finite size of our model space (Schottky effect), the peak at  $T = 0.2$  MeV is a unique structure of odd-odd  $N = Z$  nuclei with  $A > 40$  (except for  $^{58}\text{Cu}$ ). As we pointed out earlier, these nuclei have ground state isospins  $T = 1$  and  $J = 0$ , and exhibit, like their even-even analogs  $^{46}\text{Ti}$  and  $^{46}\text{Cr}$ , a sparse spectrum of  $T = 1$  levels at low energies reflecting the strong isovector pairing. However, in odd-odd  $N = Z$  nuclei the lowest levels with  $T = 0$  and  $T = 1$  are almost degenerate reflecting a competition of pairing and symmetry energy. Furthermore, as can be seen in Fig. 1, odd-odd  $N = Z$  nuclei exhibit several  $T = 0$  levels at low excitation energy and these levels have  $J > 0$ .

The peak in the specific heat at  $T = 0.2$  MeV signals the “transition” from the  $T = 1$  ground state to the bunch of  $T = 0$  levels (with larger statistical weight) at low excitation energy. We note that the peak will be somewhat shifted towards higher temperatures if we add an attractive component  $b\hat{T}^2$ , with the isospin operator  $\hat{T}$ , to the Hamiltonian to correct for the slight mismatch between the  $T = 1$  and  $T = 0$  levels in our calculation. In passing we also remark that such a peak is not visible in the specific heat for odd-odd  $N = Z$  nuclei with  $T = 0$  ground states and angular momenta  $J > 0$ , where the  $T, J = 1, 0$  level is at a modest excitation energy and due to its small statistical weight does not show up as peak in the specific heat.

To complete our discussion of the  $^{46}\text{V}$  spectrum we have plotted the level density in Fig. 3. For clarity we have binned the results in 0.5 MeV bins and exhibit them for both isospin channels  $T = 0$  and  $T = 1$  separately. As is customary, we compare our shell model level densities with the backshifted Fermi gas [23].

$$\rho(U) = \frac{\sqrt{\pi}}{12a^{1/4}} \frac{\exp 2\sqrt{aU}}{U^{5/4}}; \quad U = E - \Delta \quad (3)$$

where  $\Delta, a$  are the backshift and level density parameter, respectively. These two essential parameters of the model are determined by global fits to experimental data at low energies (around the neutron threshold and below), leading to the approximate expressions [23]

$$a \approx A/8 \text{ MeV}^{-1} \quad (4)$$

$$\Delta \approx \pm \frac{12}{\sqrt{A}} - \frac{10}{A} \text{ MeV} \quad (5)$$

with the positive (negative) sign for even-even (odd-odd) nuclei and  $\Delta = 0$  for odd- $A$  nuclei. We note that the experimentally determined value of  $a$  is significantly larger than the Fermi gas value ( $a \approx A/16 \text{ MeV}^{-1}$ ) indicating the presence of additional correlations in the low-energy levels other than those described by pairing. The calculated  $^{46}\text{V}$  level density is reasonably well described in the energy regime  $E > 2.5 \text{ MeV}$  by the backshifted Fermi gas model with the parameters  $\Delta = -2.0 \text{ MeV}$  and  $a = 3.5 \text{ MeV}^{-1}$ . While  $\Delta$  agrees well with the empirical value, our  $a$  is significantly smaller suggesting the presence of states outside of our model space in  $^{46}\text{V}$  already at rather low excitation energies. The discrepancy in  $a$  is less than the comparison with Eq. (4) suggests; in Ref. [24] the values  $\Delta = -1.79 \text{ MeV}$  and  $a = 4.9 \text{ MeV}^{-1}$  are recommended, closer to the ones found here.

As we have seen already in the discussion of the spectrum, pairing plays an essential role. We will now investigate this topic in more detail by studying the pair correlation strength in  $^{46}\text{V}$  as a function of excitation energy. We restrict our discussion to  $s$ -wave pairing only, hence  $L = 0$ . As a measure of the pair correlation strength we use the operator  $\mathcal{N}_{JTt_z}$ , defined in  $LS$ -coupling by:

$$\mathcal{N}_{JTt_z} = \sum_{ll'M} \sqrt{(2l+1)(2l'+1)} A_{0SJ M}^{Tt_z \dagger}(ll) A_{0SJ M}^{Tt_z}(l'l') \quad (6)$$

with the two particle creation operator  $A^\dagger$ :

$$A_{LSJM}^{Tt_z \dagger}(l_A l_B) = \frac{1}{\sqrt{1+\delta_{AB}}} \left[ a_A^\dagger a_B^\dagger \right]_{LSJM}^{Tt_z}. \quad (7)$$

and  $a_{nlms_z t_z}^\dagger$  creates a nucleon of isospin projection  $t_z$  and spin projection  $s_z$  in the orbital  $nlm$ . In our studies involving the diagonalization approach the expectation value is evaluated state-by-state. In the SMMC approach the expectation value refers to a thermal average defined as

$$\langle \mathcal{O} \rangle = \frac{\text{Tr}_A \exp[-\beta H] \mathcal{O}}{Z} \quad (8)$$

where  $\text{Tr}_A$  is the canonical trace (fixed numbers of neutrons and protons) and  $H$  is the many-body Hamiltonian.

In the limit of large degeneracy  $\langle \mathcal{N} \rangle$  represents the number of nucleon pairs with the angular momentum  $J$ , isospin  $T$  and its projection  $t_z$ . In  $pf$  shell nuclei the degeneracies are not too large, the operators  $A, A^\dagger$  are not really bosons, and hence  $\langle \mathcal{N}_{t_z} \rangle$  can deviate from the true pair number expectation value.

Fig. 4 shows the isovector ( $T = 1, S = 0$ ) and isoscalar ( $T = 0, S = 1$ ) pair correlation strength as function of excitation energy (averaged in  $0.5 \text{ MeV}$  wide bins) and for  $T = 0$  and  $T = 1$  states in  $^{46}\text{V}$  separately. Isospin symmetry requires  $\langle \mathcal{N}_{J=0, T=1, t_z} \rangle$  to be identical for all three isovector channels ( $pp$ ,  $nn$ ,  $pn$ ) in  $T = 0$  states, while isovector  $pn$  pairing can be different from like-particle

pairing in the  $T = 1$  states ( $pp$  and  $nn$  pairing strengths are still identical). Several observations with respect to Fig. 4 are noteworthy: Isovector pairing dominates in both  $T = 0$  and  $T = 1$  states at low excitation energies. With the exception of the states below  $1 \text{ MeV}$ , isovector pairing decreases, approximately exponentially, in  $T = 0$  states with energy. On the other hand, the isoscalar pairing in  $T = 0$  states is about constant up to  $E = 6 \text{ MeV}$  and then decreases more slowly than isovector pairing. We conclude that isovector pairing in  $T = 0$  states is more concentrated in the low-energy part of the spectrum, while isoscalar pairing is also present at higher energies. The difference is, as stated earlier and shown in detail below, presumably due to spin-orbit splitting, which introduces an additional energy scale into the isoscalar  $pn$  pairing mode ( $\epsilon_{7/2} - \epsilon_{5/2} \approx 6 \text{ MeV}$ ) which is only overcome at higher energies.

The lowest  $T = 1$  states are dominated by isovector  $pn$  pairing. In these states, like-particle pairing is roughly constant, in fact it increases slightly with energy. We conclude that the isovector pairing gap in  $^{46}\text{V}$  is due to  $pn$  pairing. For states with  $E^* > 4 \text{ MeV}$ , when the “pairing gap” is overcome, we find no large difference between the three isovector pairing correlation strengths. While the sum of isovector pairing is still larger than the isoscalar pairing strength, the latter is stronger than each of the three individual channels. As for  $T = 0$  states, isoscalar pairing decreases more slowly than isovector pairing and becomes the largest correlation for  $E^* > 15 \text{ MeV}$  (however, at these high excitation energies our model space is quantitatively not adequate anymore and should be extended to include the two neighboring major shells).

What is the origin of the pairing correlations? It is wellknown that a “realistic” shell model interaction can be approximated by a monopole term and a two-body piece consisting of pairing and quadrupole-quadrupole ( $QQ$ ) terms (Bes-Sorensen interaction [25]). Thus the correlation can reflect both genuine pairing interaction or deformation which is related to the  $QQ$  interaction. To distinguish between these different sources we define first the total correlation energy  $H_{corr}$  by subtracting the monopole contribution that includes both single particle energies and average two body matrix elements [26] from the expectation value of the full Hamiltonian. Next, we measure the importance of the two dominating pieces in the residual interaction by calculating the expectation values of the pairing,  $H_{\text{pair}}$ , and quadrupole-quadrupole,  $H_{QQ}$ , hamiltonians in the eigenstates of the full Hamiltonian. These Hamiltonians are defined by

$$H_{\text{pair}} = -G_{p01} \sum_{t_z} \mathcal{N}_{01t_z} - G_{p10} \mathcal{N}_{100}, \quad (9a)$$

$$H_{QQ} = -\chi \sum_{\mu} (-1)^{\mu} Q_{\mu} Q_{-\mu}, \quad (9b)$$

where  $Q_{\mu}$  is the mass quadrupole operator defined as:

$$Q_\mu = \sqrt{\frac{16\pi}{5}} \sum_i^A r_i^2 Y_{2\mu}(\Omega_i). \quad (9c)$$

The values of the different constants are taken from table II of reference [27]. After scaling to the corresponding  $\hbar\omega$  the values are:  $G_{p01} = 0.37$  MeV,  $G_{p10} = 0.57$  MeV, and  $\chi = 0.014$  MeV. The expectation values are shown in Fig. 5 as a function of temperature. We have additionally split them into their isovector and isoscalar components defined by taking the isovector and isoscalar pieces of the respective Hamiltonians when they are written in the normal order. The results support the discussion given above. The isovector correlation energy is stronger than the isoscalar one. At the same time, while the isoscalar correlation energy decreases gradually and slowly, there is a noticeable drop in the isovector correlation energy at low temperatures which can be traced back to the pairing. In the ground state (temperature  $T = 0$ ) most of the correlation energy is due to pairing energy, but the expectation value of the isovector component of the pairing Hamiltonian has dropped to about half of its ground state value already at temperature  $T = 0.25$  MeV. By splitting  $H_{pair}$  into its various components, we verify that most of the isovector pairing energy (about 60%) and its drop with temperature is caused by proton-neutron pairing.

Strikingly the isoscalar pairing correlation energy decreases very slowly. While the results for the isovector pairing correlation energy confirms the expectation and shows that this degree of freedom is mainly concentrated in states at low excitation energies, our calculation suggests that a well pronounced “pairing gap” does not exist in isoscalar pairing. This conclusion is based on the comparison of the isovector and isoscalar pair correlation energies in Fig. 5; there is no peak at low energies in the  $T = 0$  channel. (The apparent minimum of the  $T = 0$  level density around 2 MeV in Fig. 3 appears to be a statistical fluctuation.)

On the other hand, the isoscalar component of  $H_{QQ}$  increases slightly at small temperatures, counterbalancing the slight decrease in the isoscalar piece of  $H_{pair}$ . The isovector component of  $H_{QQ}$  is roughly constant in the temperature regime  $T < 0.25$  MeV, which is dominated by the states with large isovector pairing contributions. We also notice that the isoscalar quadrupole-quadrupole correlations decrease more slowly than the isovector ones.

In Figure 6 we compare the values of the different correlations obtained by adding the isoscalar and isovector parts. Clearly pairing plus quadrupole accounts for most of the total correlation energy as measured by  $H_{corr}$ . The contributions of the other components of the nuclear force (see [27] for a complete characterization) are practically independent of the temperature. We note that at  $T \approx 0.15$  MeV, where the peak in the specific heat in figure 2 appears, the quadrupole correlations became dominant over pairing correlations as the low lying  $T = 0$  states, that dominate the thermal average at this temperatures, have bigger quadrupole energies than pairing energies.

Finally, we like to report on SMMC calculations of the even Fe-nuclei  $^{50-58}\text{Fe}$ . We have chosen this set of isotopes as it includes an  $N = Z$  nucleus ( $^{52}\text{Fe}$ ), a closed-shell nucleus ( $^{54}\text{Fe}$ ), and nuclei with valence protons and neutrons in different subshells ( $^{56,58}\text{Fe}$ ). Our calculation parallels the SMMC study in Ref. [2] where the reader might find details about the approach. Parts of the results concerning pairing have already been presented in Ref. [2], although in different context.

To distinguish between genuine pair correlations and those reflecting the different number of neutrons, we introduce the excess of pair correlations  $\mathcal{N}_{exc}$  defined by subtracting the mean-field values from the pair correlation strength defined in Eq. (6). Following Ref. [19] we define the mean-field value by the uncorrelated Fermi gas value using the factorization

$$\langle a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta \rangle = n_\beta n_\alpha (\delta_{\beta\gamma} \delta_{\alpha\delta} - \delta_{\beta\delta} \delta_{\alpha\gamma}) \quad (10)$$

where  $n_\alpha$  are the occupation numbers. Fig. 7 shows the excess of isovector and isoscalar pair correlations. Furthermore we have indicated which orbital coupling mainly contribute to these excesses.

Isovector  $pn$  correlations are strongest in the  $N = Z$  nucleus  $^{52}\text{Fe}$  and decrease rapidly with increasing  $|N - Z|$ . This result confirms the general trend already outlined in [1] which noticed that with increasing  $|N - Z|$  nuclear ground states show the tendency to split into separate proton and neutron condensates. The decreasing  $pn$  correlations also allow an increase in  $pp$  correlation with growing  $|N - Z|$ , as can be also seen in Fig. 7. The excess of  $nn$  correlations, however, does not follow the simple SO(5) picture as shell effects, which are not present in that model, play an essential role. One clearly observes that  $\mathcal{N}_{exc}$  decreases strongly towards the magic neutron number  $N = 28$  reflecting the closure of the  $f_{7/2}$  shell in  $^{54}\text{Fe}$ . With two neutrons outside of  $f_{7/2}$  neutron correlations increase again ( $^{56}\text{Fe}$ ), but are somewhat reduced again in  $^{58}\text{Fe}$  due to the partly closure of the  $p_{3/2}$  subshell. For this nucleus most of the  $nn$  correlations are due to pairing in the  $f_{5/2}$  and  $p_{1/2}$  orbitals.

A closer inspection of the  $pp$  correlations indicates that the  $f_{5/2}$  orbitals contribute more than the  $p_{3/2}$  orbitals, although the latter are energetically favored. This is already a signal for the presence of the isoscalar  $pn$  pairing which introduces  $f_{7/2} - f_{5/2}$  correlations which are roughly the same for all investigated Fe-isotopes. As long as the  $f_{7/2}$  neutron shell is not filled, we also find isoscalar  $pn$  correlations among the  $f_{7/2}$  orbitals. For the heavier isotopes these correlations are actually smaller than the mean-field values indicating that other correlations become more important.

As suggested above, isoscalar  $pn$  correlations are expected to be sensitive to the amount of spin-orbit splitting. To quantify this statement we have repeated our SMMC studies of  $^{50}\text{Fe}$  and  $^{56}\text{Fe}$  by artificially reducing the spin-orbit splitting in the single-particle energies by a factor of 2; thus we use  $\epsilon_{7/2} = 0.$ ,  $\epsilon_{3/2} = 2.$ ,  $\epsilon_{5/2} =$

3.,  $\epsilon_{1/2} = 3$ . As expected, the reduction of the spin-orbit splitting generally increases the isoscalar correlations at the expense of the isovector correlations. In particular, the isoscalar correlations due to the coupling of the spin-orbit partners  $f_{7/2} - f_{5/2}$  are strongly increased (by about a factor of 2.5 in these nuclei). However, a deviation from this general trend is also noteworthy. The increase of isoscalar correlations leads also to an increase of  $nn$  correlations in  $^{56}\text{Fe}$  due to increase of correlations in the  $f_{5/2}$  orbital.

Obviously coupling between  $f_{7/2}f_{5/2}$  is very strong. Will it dominate if the spin-orbit splitting were removed? Unfortunately such a calculation cannot be performed with the SMMC method due to the breakdown of the  $g$ -extrapolation [20]. For that reason we have gone back to  $^{46}\text{V}$  and have performed one shell model diagonalization study with the KB3 interaction and one in which the monopole terms have been removed from the interaction. In both cases we then calculated the expectation value of the isovector and isoscalar pairing Hamiltonians in the lowest  $T = 0$  state, which is the ground state in this academic case. For the eigenstate of the realistic Hamiltonian we find  $\langle H_{pair}^{T=1} \rangle = 2.18$  MeV and  $\langle H_{pair}^{T=0} \rangle = 1.41$  MeV, while the magnitude is inverted if the monopole terms are taken out:  $\langle H_{pair}^{T=1} \rangle = 2.09$  MeV and  $\langle H_{pair}^{T=0} \rangle = 4.62$  MeV. It is thus obvious that isovector correlations in odd-odd  $N = Z$  nuclei win over isoscalar correlations due to the presence of the spin-orbit splitting.

### III. CONCLUSIONS

Modern diagonalization codes make it possible to study nuclear spectra state-by-state even for nuclei rather far away from closed shells, where correlations play a decisive role. Here, we use the  $N = Z$  odd-odd nucleus  $^{46}\text{V}$  as a case study for the investigation of pairing and other correlations. We are able to describe not only the ground state, but the development of various correlations with the excitation energy and, respectively, temperature.

Our main emphasis is on the competition between the two basic modes (like-particle ( $pp$  and  $nn$ ) and proton-neutron ( $pn$ )) of the isovector pairing on one hand, and the isoscalar pairing on the other hand. These features are particularly important in  $^{46}\text{V}$ , where the ground state spin and isospin  $J, T = 0, 1$  demonstrates the importance of the  $np$  isovector pairing. We show that this mode of pairing peaks sharply at low energies. At energies or temperatures above the isovector pairing gap ( $E \geq 3$  MeV or  $T \geq 0.5$  MeV) the three isovector pairing strengths become essentially equal to each other, and gradually decrease. At the same time, the isoscalar pairing energy, which is smaller than the isovector one inside the gap, becomes at higher energies comparable with the *total* isovector pairing, or even bigger.

We have shown (Fig. 2) that the large statistical

weight of the low-lying excited isospin  $T = 0$  states causes a characteristic maximum in the specific heat  $C_V$ . This feature represents an analog of the phase transition from the  $T = 1$  ground state to the regime where the partition function and internal energy are dominated by the  $T = 0$  states.

Finally, we study the contributions to the correlation energy at different temperatures in  $^{46}\text{V}$ . We show, first of all, that as expected pairing and quadrupole correlations account for most of the total correlation energy everywhere. All other correlations contribute about 2 MeV, and this amount is essentially independent of temperature. Pairing dominates near the ground state, but soon (for temperatures above 250 keV) pairing and quadrupole correlation energies become comparable.

In an additional study based on the SMMC we show how pair correlations in Fe isotopes depend on  $|N - Z|$ . In particular, we were able to trace the contribution of individual subshells to the pairing strength. That calculation also confirmed that the isovector  $pn$  pairing strength decreases fast with increasing  $|N - Z|$ . On the other hand, the isoscalar  $pn$  pairing in this chain of isotopes is almost independent on  $|N - Z|$ .

In the  $\text{SU}(4)$  limit, i.e. for degenerate single particle levels, identical coupling constant of the isoscalar and isovector pairing force and absence of other components in the residual interaction, the lowest  $T = 0$  and  $T = 1$  states are degenerate. However, these symmetries are lifted in realistic cases and, for the present nucleus  $^{46}\text{V}$ , the ground state has  $T = 1$ . At first we note that the coupling constant of the isoscalar and isovector pairing force, determined in Ref. [27], are  $G_{p01} = 0.37$  MeV, and  $G_{p10} = 0.57$  MeV, i.e. the isoscalar pairing is stronger. Why does the isovector pairing nevertheless dominate the ground state? We argued that the effect of the isoscalar pairing is weakened by the spin-orbit splitting which introduces additional energy scale into the problem. The isoscalar pairing can act efficiently only at energies where the spin-orbit splitting plays only a minor role. To prove that point we have artificially reduced the spin orbit splitting in Fe isotopes, and indeed observed an increase of the isoscalar pairing. But through higher order effects the isovector pairing was affected as well. Furthermore, we have shown that in the lowest  $T = 0$  state in  $^{46}\text{V}$  the isoscalar correlations would prevail if the spin-orbit force were switched off. Thus, this somewhat academic exercise has confirmed to us that without the strong spin-orbit force the nuclear ground states would look very differently from the ones we are familiar with.

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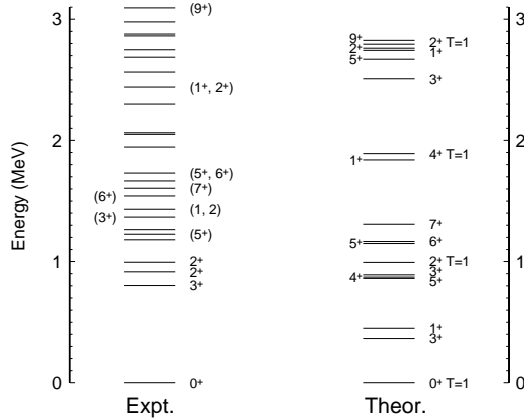


FIG. 1. Calculated and experimental spectra of  $^{46}\text{V}$ . Only the isospin of the ground state is known experimentally. The energies of the excited  $T=1$  states in  $^{46}\text{V}$  can be estimated from the isobaric analog states in  $^{46}\text{Ti}$ :  $2^+$  (0.889 MeV),  $4^+$  (2.010 MeV),  $0^+$  (2.611 MeV),  $2^+$  (2.962 MeV).

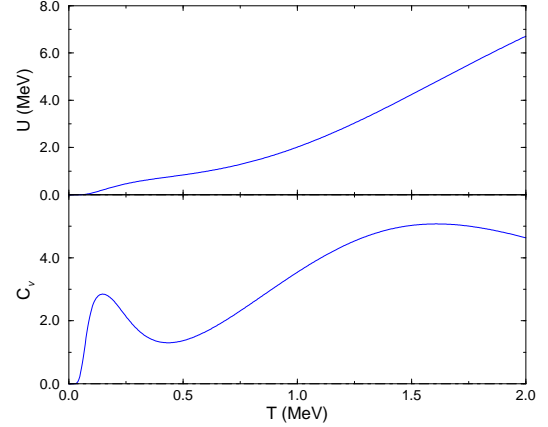


FIG. 2. Internal energy  $U$  (upper panel) and specific heat  $C_V$  (lower panel) of  $^{46}\text{V}$  as a function of temperature  $T$ .

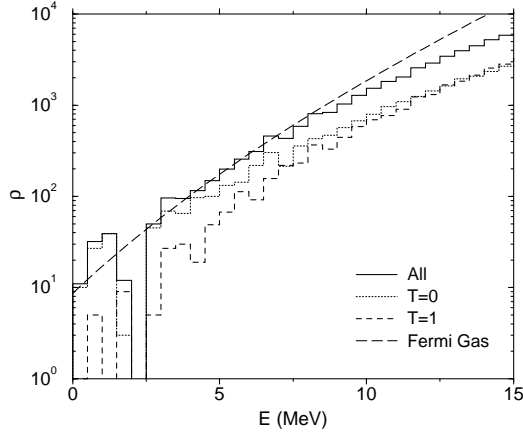


FIG. 3. Level density of  $^{46}\text{V}$  as function of the excitation energy. The levels with isospin  $T=0$  and 1 are shown separately. The Fermi gas level density parameters were  $a = 3.5 \text{ MeV}^{-1}$  and  $\Delta = -2.0 \text{ MeV}$ .

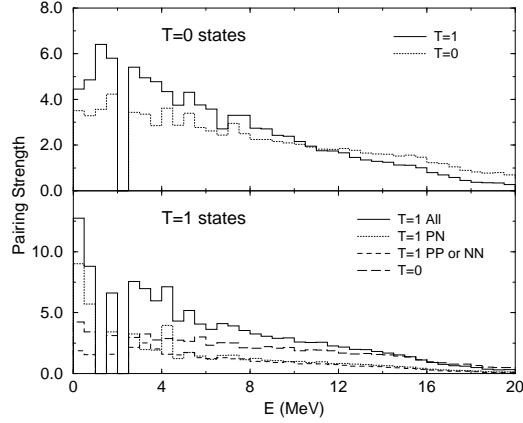


FIG. 4. Average isovector  $T = 1, S = 0, L = 0$  and isoscalar  $T = 0, S = 1, L = 0$  pair correlation strengths in  $^{46}\text{V}$  as function of the excitation energy (binned for clarity in bins 0.5 MeV wide).

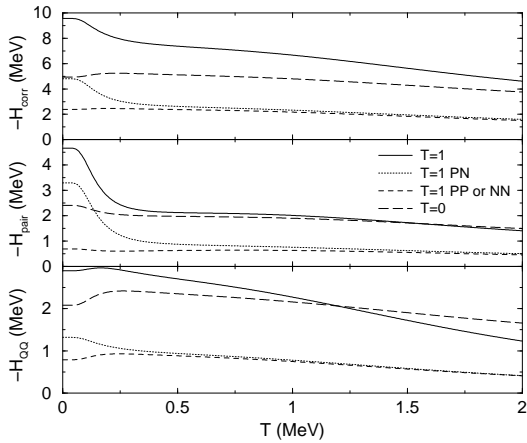


FIG. 5. Expectation values of the total correlation energy, isoscalar and isovector parts of pairing, and quadrupole-quadrupole energies as a function of the temperature for  $^{46}\text{V}$ .

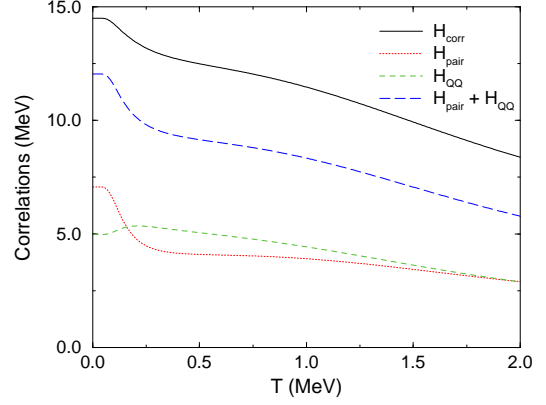


FIG. 6. Expectation values of the pairing, quadrupole-quadrupole and total correlation energies as a function of the temperature for  $^{46}\text{V}$ .

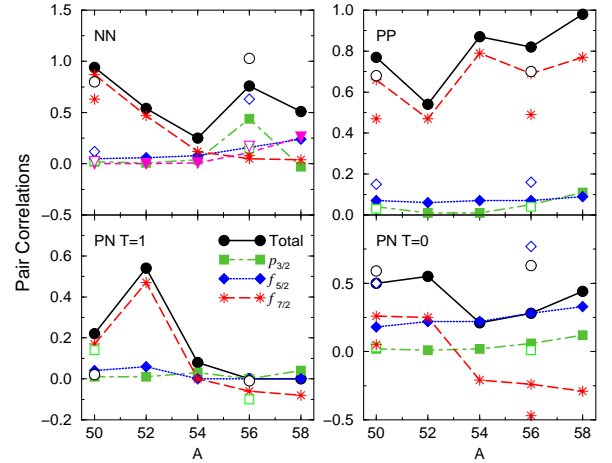


FIG. 7. Isovector and isoscalar pairing correlation in Fe isotopes. The excess over the mean field value is plotted. The unfilled symbols refer to the SMMC studies of  $^{50}\text{Fe}$  and  $^{56}\text{Fe}$ , in which we have artificially halved the spin-orbit splitting in the single particle energies (see text).